Distillation Blending and Cutpoint Temperature Optimization using Monotonic Interpolation

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Kelly, Menezes & Grossmann, 2014
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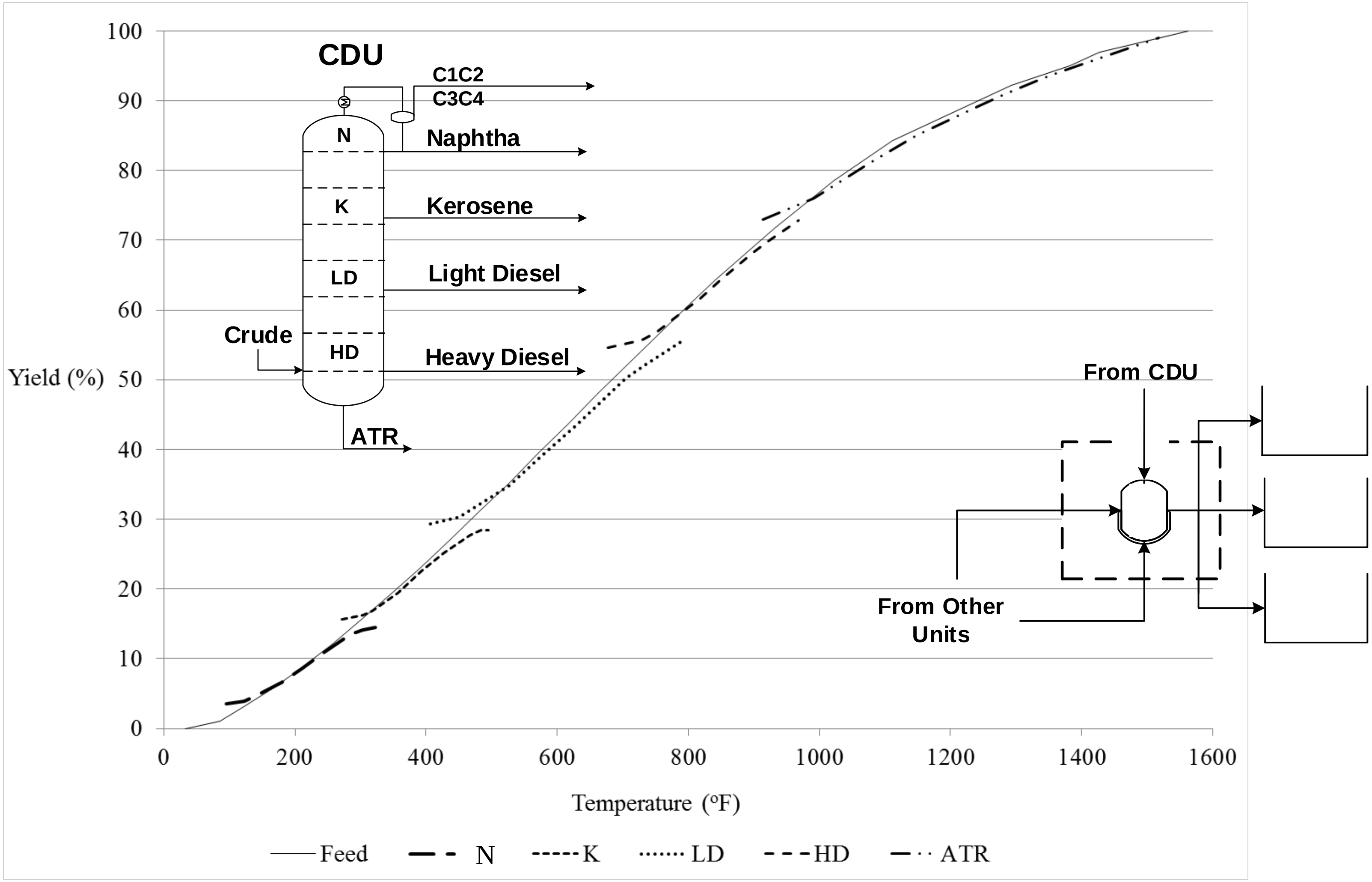
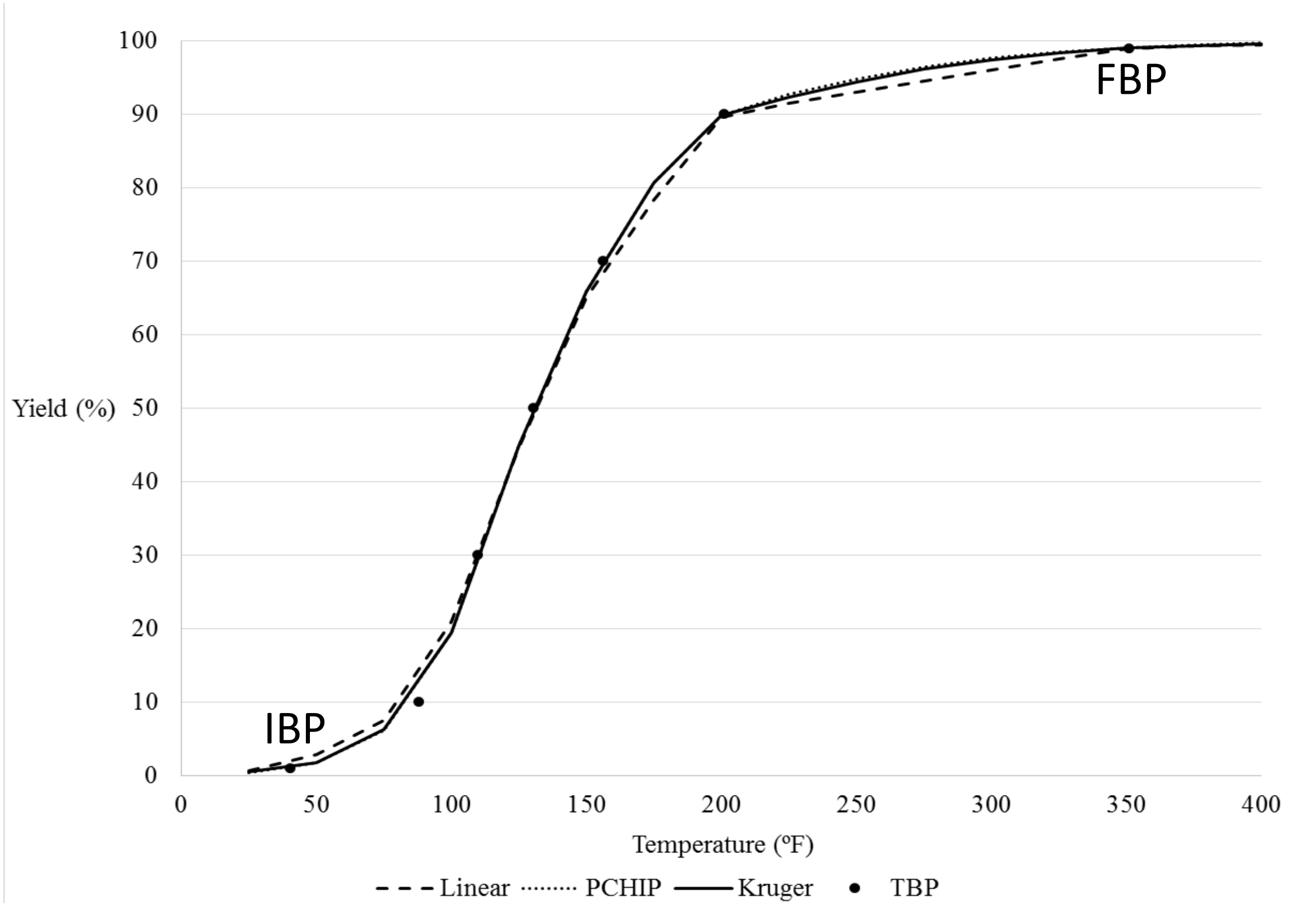
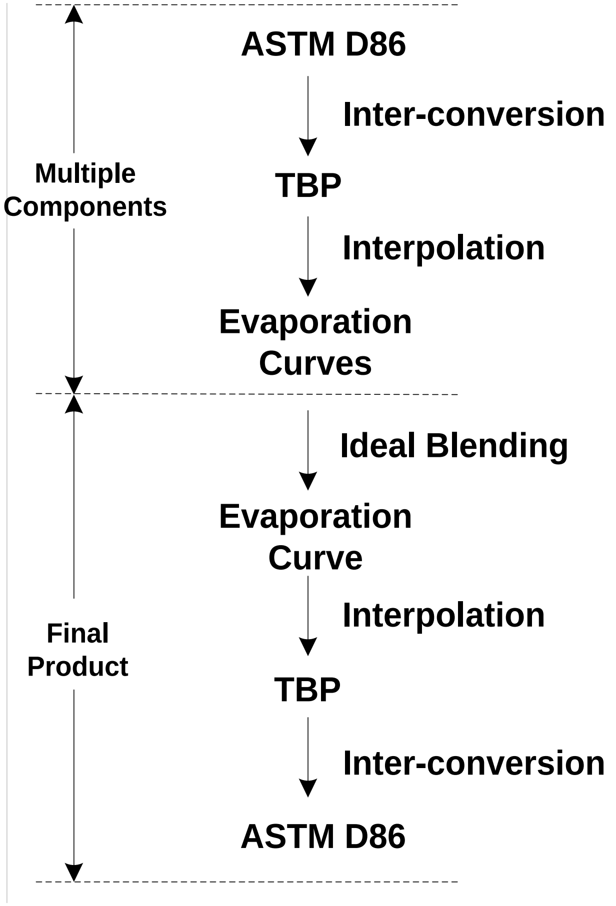
Goal: integrate blending of several streams’ distillation curves together with also shifting or adjusting the cutpoints of one or more of the distilled stream’s initial and/or final boiling-points (IBP and FBP) in order to manipulate its TBP curve in an either off- or on-line environment.



ASTM D86 – TBP Inter-conversion

Methodology: inter-convert from ASTM D86 to TBP temperatures where the blending component are mixed using the ideal blending law and then interpolate the points into evaporation curves using monotonic interpolation (Linear, PCHP, or Kruger).





Multiple Components

ASTM D86

Inter-conversion

TBP

Interpolation

Evaporation Curves

Final Product

Ideal Blending

Evaporation Curve

Interpolation

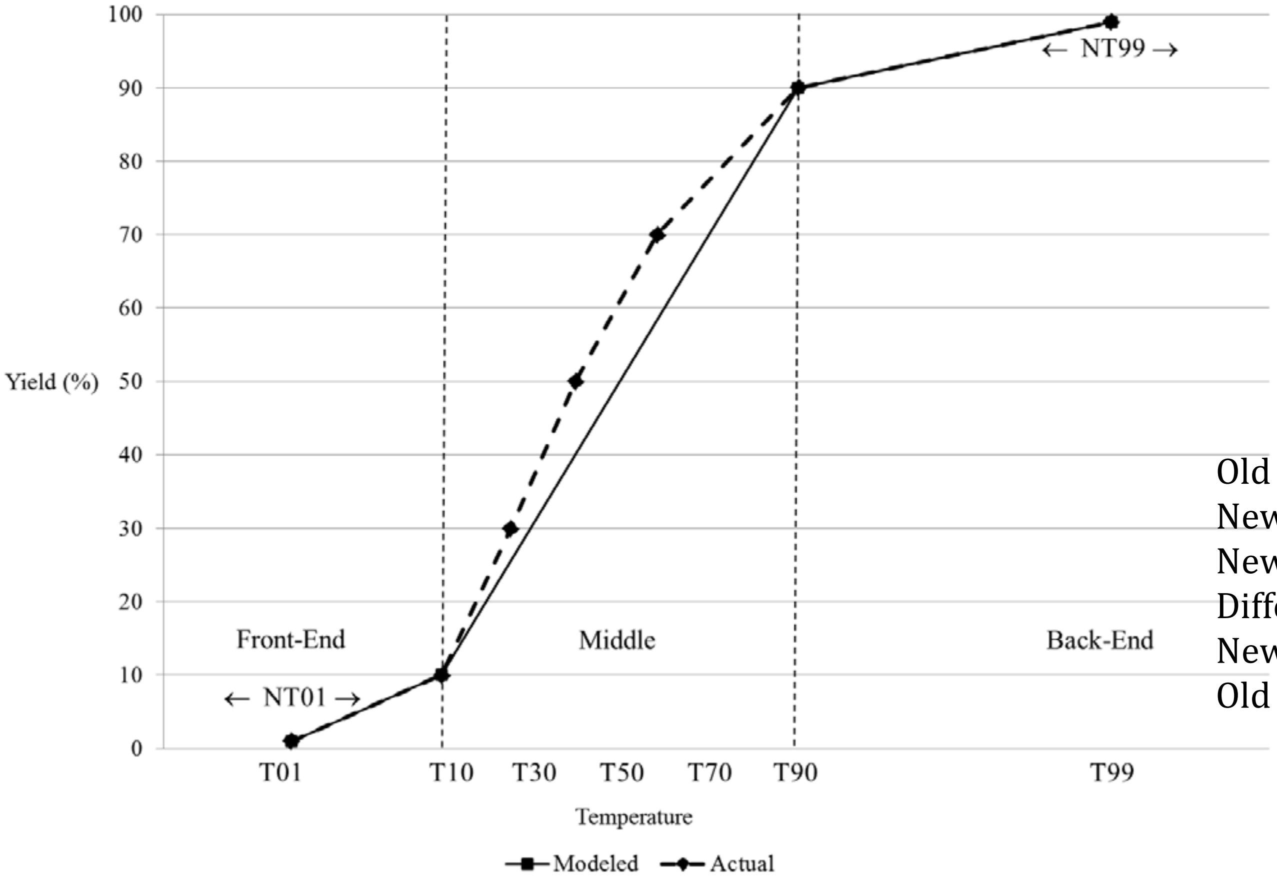
TBP

Inter-conversion

ASTM D86

Distillation curve adjustment or shifting technique

A typical distillation curve can be reasonably decomposed or partitioned into three distinct regions or parts i.e., *a front-end, middle and back-end*.



Old Temperature: OT
New Temperature: NT
New Yield: YNT
Difference in Yield: DYNT
New Flow: NF
Old Flow: OF (measured)

$$\mathrm{YNT01} = 0.10 - \frac{0.10-0.01}{\mathrm{OT10}-\mathrm{OT01}}(\mathrm{OT10}-\mathrm{NT01})$$

$$\mathrm{YNT99} = 0.90 + \frac{0.99-0.90}{\mathrm{OT99}-\mathrm{OT90}}(\mathrm{NT99}-\mathrm{OT90})$$

$$\left.\begin{array}{l} \mathrm{DYNT01} = 0.01 - \mathrm{YNT01} \\ \\ \mathrm{DYNT99} = \mathrm{YNT99} - 0.99 \end{array}\right\} \mathrm{NF} = \mathrm{OF}(1 + \mathrm{DYNT01} + \mathrm{DYNT99})$$

Relative Yields Normalization

Given the IBP and FBP delta yield amounts $\mathrm{DYNT01}$ and $\mathrm{DYNT99}$, can easily adjust new yields, given the old yields, i.e. the well-defined 1%, 10%, 30%, etc. values.

$$
\begin{aligned}
\mathrm{NY01} &= 0.01/(1+\mathrm{DYNT99})\\
\mathrm{NY10} &= (0.10+\mathrm{DYNT01})/(1+\mathrm{DYNT01}+\mathrm{DYNT99})\\
\mathrm{NY30} &= (0.30+\mathrm{DYNT01})/(1+\mathrm{DYNT01}+\mathrm{DYNT99})\\
\mathrm{NY50} &= (0.50+\mathrm{DYNT01})/(1+\mathrm{DYNT01}+\mathrm{DYNT99})\\
\mathrm{NY70} &= (0.70+\mathrm{DYNT01})/(1+\mathrm{DYNT01}+\mathrm{DYNT99})\\
\mathrm{NY90} &= (0.90+\mathrm{DYNT01})/(1+\mathrm{DYNT01}+\mathrm{DYNT99})\\
\mathrm{NY99} &= (0.99+\mathrm{DYNT01})/(1+\mathrm{DYNT01}+\mathrm{DYNT99})
\end{aligned}
$$

Cutpoint is somewhat different in this work than Mahalec and Sanchez (2012) and Menezes, Kelly and Grossmann (2013): *middle point of the final and initial boiling point temperatures of adjacent streams.*

Since the TBP curve of a CDU’s crude-oil mixture is not normally available, we use the definition commonly found in oil-refinery operations of defining ***Cutpoint temperatures smallest and/or largest controllable separation or fractionation temperature (i.e., IBP, 5% or 10%, and 90%, 95%, or FBP) between adjacent cuts, fractions, or streams from a distillation tower.***

Example

- Solved using **IMPL** (Industrial Modeling and Programming Language) from Industrial Algorithms LLC that implements monotonic interpolation as standard built-in functions. All first-order partial derivatives are computed numerically, but close to analytical quality, and **automatically** for the variables found in both the abscissa and ordinate axes of the interpolation dataset.

Example: *Maximize flow of DC1 and DC2 subject to relative and arbitrary pricing of 0.9 for DC1 and 1.0 DC2 with lower and upper bounds of 0.0 and 100.0 each*
Flows for DC3 and DC4 are fixed to a marginal and arbitrary value of 1.0 and the total blend flow cannot exceed 100.0 and its ASTM D86 specifications are D10 ≤ 470, 540 ≤ D90 ≤ 630 and D99 ≤ 680. (DC = diesel component)

Table. Inter-Converted TBP (ASTM D86) Temperatures in Degrees F.

	DC1	DC2	DC3	DC4
1%	305.2 (353)	322.2 (367)	327.0 (385)	302.4 (368)
10%	432.9 (466)	447.1 (476)	405.2 (435)	369.7 (407)
30%	521.6 (523)	507.1 (509)	457.1 (462)	441.0 (449)
50%	565.3 (551)	549.5 (536)	503.3 (492)	513.8 (502)
70%	606.4 (581)	598.4 (573)	551.1 (528)	574.3 (550)
90%	668.3 (635)	666.1 (634)	605.8 (574)	625.4 (592)
99%	715.7 (672)	757.7 (689)	647.0 (608)	655.2 (620)

Example

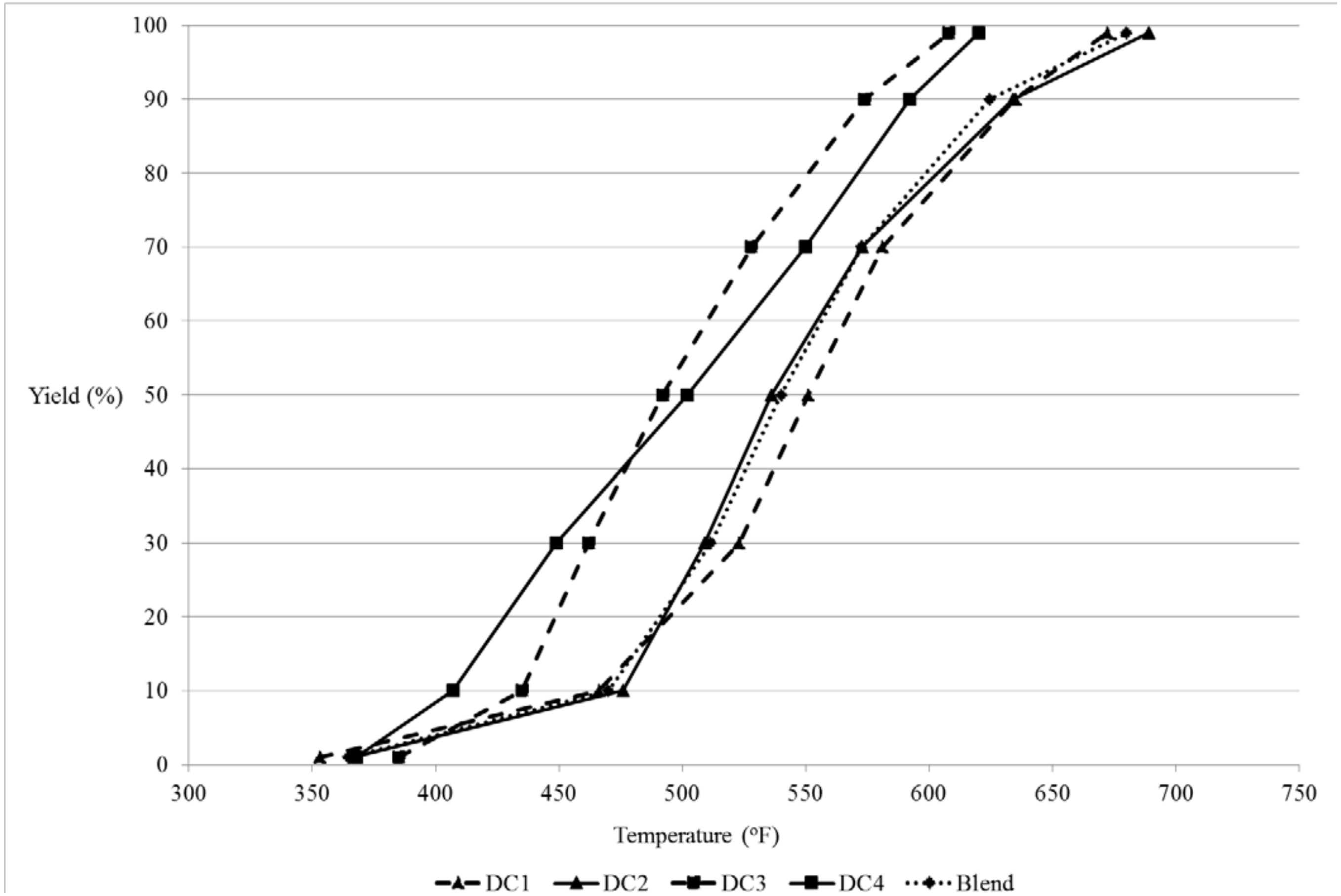


Figure. ASTM D86 distillation curves, including the final blend, which is determined by the blended TBP interconversion to ASTM D86.

The new and optimized TBP curve for DC1 given its front and back-end shifts is now [(1.053%,312.8), (10.015%,432.9), (31.188%,521.6), (52.361%,565.3), (73.534%,606.4), (94.707%,668.3), (98.995%,689.3)]

Conclusions

Novelty:

- Integration of the distillation unit and fuel blending using IBP and FBP (cutpoints) of the streams
- Distillation curve adjustment or shifting technique considering initial, middle and final regions
- Distillation curve normalization after the new yields and cutpoint temperatures for the IBP and FBP based on the difference between the old and new yields (DYNT01 and DYNT99)
- IMPL innovation: first-order partial derivatives are computed automatically for the variables found in both the abscissa and ordinate axes of the interpolation dataset (there's no need to fit the interpolation in advance and give its derivative equation)

Conclusions

Impact for industrial applications:

- Integrate the distillation unit operation and the fuel blending
- Based on daily experimental data run gathered in the field (ASTM D86) instead of blending indices correlations
- Reduce losses by off-spec fuels
- Reduce the blender RTO efforts to get on-spec fuels